Bernard Delley

List of Publications by Year
in descending order

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81 papers	5,923 citations	101384 36 h-index	69108 77 g-index
87 all docs	87 docs citations	87 times ranked	6550 citing authors

#	Article	IF	Citations
1	Fast Calculation of Electrostatics in Crystals and Large Molecules. The Journal of Physical Chemistry, 1996, 100, 6107-6110.	2.9	860
2	Kondo Scattering Observed at a Single Magnetic Impurity. Physical Review Letters, 1998, 80, 2893-2896.	2.9	590
3	The generation and use of delocalized internal coordinates in geometry optimization. Journal of Chemical Physics, 1996, 105, 192-212.	1.2	305
4	Thermodynamic stability and structure of copper oxide surfaces: A first-principles investigation. Physical Review B, 2007, 75, .	1.1	275
5	Dissociation ofO2at Al(111): The Role of Spin Selection Rules. Physical Review Letters, 2005, 94, 036104.	2.9	259
6	Oxygen adsorption and stability of surface oxides onCu(111): A first-principles investigation. Physical Review B, 2006, 73, .	1.1	248
7	Binding energies, molecular structures, and vibrational frequencies of transition metal carbonyls using density functional theory with gradient corrections. Journal of Chemical Physics, 1994, 100, 5785-5791.	1.2	245
8	Water adsorption on the stoichiometric and reduced CeO2(111) surface: a first-principles investigation. Physical Chemistry Chemical Physics, 2009, 11, 9188.	1.3	229
9	Spin density in a nitronyl nitroxide free radical. Polarized neutron diffraction investigation and ab initio calculations. Journal of the American Chemical Society, 1994, 116, 2019-2027.	6.6	228
10	Gas-phase-dependent properties ofSnO2(110), (100), and (101) single-crystal surfaces: Structure, composition, and electronic properties. Physical Review B, 2005, 72, .	1.1	211
11	Stability and morphology of cerium oxide surfaces in an oxidizing environment: A first-principles investigation. Journal of Chemical Physics, 2009, 131, .	1.2	150
12	Superhard Nitride-Based Nanocomposites: Role of Interfaces and Effect of Impurities. Physical Review Letters, 2006, 97, 086102.	2.9	122
13	Evidence for Transmission of Ferromagnetic Interactions through Hydrogen Bonds in Alkyne-Substituted Nitroxide Radicals:Â Magnetostructural Correlations and Polarized Neutron Diffraction Studies. Journal of the American Chemical Society, 2000, 122, 1298-1309.	6.6	109
14	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mr Physical Review B, 2009, 79, .	1.1	109
15	Geometry and diameter dependence of the electronic and physical properties of GaN nanowires from first principles. Physical Review B, 2008, 77, .	1.1	88
16	Nonadiabatic potential-energy surfaces by constrained density-functional theory. Physical Review B, 2007, 75, .	1.1	85
17	Photogeneration of two metastable NO linkage isomers with high populations of up to 76% in trans-[RuCl(py)4(NO)][PF6]2Â·Â½H2O. Physical Chemistry Chemical Physics, 2007, 9, 3717-3724.	1.3	76
18	Bridging Hydroxyl Groups in Faujasite:Â Periodic vs Cluster Density Functional Calculations. Journal of Physical Chemistry A, 1999, 103, 3772-3777.	1.1	73

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19	Structure and properties ofTiN(111)âˆ•SixNyâˆ•TiN(111)interfaces in superhard nanocomposites: First-principles investigations. Physical Review B, 2006, 74, .	1.1	69
20	Spin Density Maps for the Ferrimagnetic Chain Compound MnCu(pba)(H2O)3Â·2H2O (pba =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 American Chemical Society, 1997, 119, 3500-3506.	6.6	67
21	[Ru(py)₄Cl(NO)](PF₆)₂Â·0.5H₂O: a model system for structural determination and ab initio calculations of photo-induced linkage NO isomers. Acta Crystallographica Section B: Structural Science, 2009, 65, 612-623.	1.8	65
22	Surface structure of Sn-doped In₂O₃(111) thin films by STM. New Journal of Physics, 2008, 10, 125030.	1.2	64
23	Long-lived light-induced metastable states in trans-[Ru(NH3)4(H2O)NO]Cl3Â·H2O and related compounds. Physical Chemistry Chemical Physics, 2005, 7, 1164-1170.	1.3	62
24	Questioning the existence of a unique ground-state structure for Si clusters. Physical Review B, 2007, 75, .	1.1	62
25	Surface oxides of the oxygenâ€“copper system: Precursors to the bulk oxide phase?. Surface Science, 2007, 601, 5809-5813.	0.8	60
26	Spectroscopic and theoretical studies of metal cluster complexes. Part 2. X.alpha. calculations and spectroscopic studies of triruthenium and triosmium dodecacarbonyls. Inorganic Chemistry, 1982, 21, 2247-2253.	1.9	58
27	Spin-Density Maps for an Oxamido-Bridged Mn(II)Cu(II) Binuclear Compound. Polarized Neutron Diffraction and Theoretical Studies. Journal of the American Chemical Society, 1996, 118, 11822-11830.	6.6	56
28	The effect of grid quality and weight derivatives in density functional calculations. Journal of Chemical Physics, 1994, 101, 8894-8902.	1.2	55
29	High order integration schemes on the unit sphere. Journal of Computational Chemistry, 1996, 17, 1152-1155.	1.5	51
30	Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111). Physical Review B, 2008, 78, .	1.1	51
31	Light harvesting with multiwall carbon nanotube/silicon heterojunctions. Nanotechnology, 2011, 22, 115701.	1.3	47
32	Quantum Chemical Analysis of Electronic Structure and n- and p-Type Charge Transport in Perfluoroarene-Modified Oligothiophene Semiconductors. Journal of Physical Chemistry B, 2006, 110, 24361-24370.	1.2	46
33	Role of oxygen inTiN(111)âˆ•SixNyâˆ•TiN(111)interfaces: Implications for superhard nanocrystallinencâˆ’TiNâˆ•aâˆ’Si3N4nanocomposites. Physical Review B, 2006, 74, .	1.1	45
34	Massive thermostatting in isothermal density functional molecular dynamics simulations. Journal of Chemical Physics, 2003, 119, 2481-2487.	1.2	39
35	Nitrogen adsorption and thin surface nitrides on Cu(111) from first-principles. Surface Science, 2007, 601, 4775-4785.	0.8	39
36	Mn-dopedCuGaS2chalcopyrites: Anab initiostudy of ferromagnetic semiconductors. Physical Review B, 2002, 66, .	1.1	38

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37	Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation. Physical Review B, 2008, 77, .	1.1	38
38	Generation of one light-induced metastable nitrosyl linkage isomer in [Pt(NH3)4Cl(NO)]Cl2 in the red spectral range. Physical Chemistry Chemical Physics, 2007, 9, 5149.	1.3	37
39	Dissociation of Water on Anatase TiO2 Nanoparticles: the Role of Undercoordinated Ti Atoms at Edges. Journal of Physical Chemistry C, 2009, 113, 15862-15867.	1.5	36
40	Electronic structure of endohedral fullerenes An@C28 (An=Th â€“ Md). Computational and Theoretical Chemistry, 2012, 985, 46-52.	1.1	36
41	Electronic structure and oxygen vacancies in PdO and ZnO: validation of DFT models. Physical Chemistry Chemical Physics, 2011, 13, 15947.	1.3	35
42	Tunable conductivity and conduction mechanism in an ultraviolet light activated electronic conductor. Journal of Applied Physics, 2005, 97, 103713.	1.1	34
43	Reversible photoswitching between nitrito-N and nitrito-O isomers in trans-[Ru(py)4(NO2)2]. Physical Chemistry Chemical Physics, 2010, 12, 6171.	1.3	33
44	Environment-dependent nanomorphology of TiN: the influence of surface vacancies. Nanoscale, 2012, 4, 5183.	2.8	32
45	Reaction intermediates of methanol synthesis and the waterâ€“gas-shift reaction on the ZnO(0001) surface. Surface Science, 2010, 604, 1742-1751.	0.8	29
46	Gap opening in the surface electronic structure of graphite induced by adsorption of alkali atoms: Photoemission experiments and density functional calculations. Physical Review B, 2005, 71, .	1.1	24
47	Photogeneration of metastable side-on N2 linkage isomers in [Ru(NH3)5N2]Cl2, [Ru(NH3)5N2]Br2 and [Os(NH3)5N2]Cl2. Physical Chemistry Chemical Physics, 2008, 10, 5531.	1.3	24
48	Why does bromine square palladium off? An ab initio study of brominated palladium and its nanomorphology. Physical Chemistry Chemical Physics, 2014, 16, 18570-18577.	1.3	24
49	Combined Ab Initio Total Energy Density Functional Calculations and Scanning Tunneling Microscopy Experiments of the Î²-SiC(001) c(4x2) Surface. Materials Science Forum, 1998, 264-268, 379-382.	0.3	22
50	A first-principles study of ultrathin nanofilms of MgO-supported TiN. Physical Chemistry Chemical Physics, 2012, 14, 2462.	1.3	22
51	Photogeneration of Nitrosyl Linkage Isomers in Octahedrally Coordinated Platinum Complexes in the Red Spectral Range. Inorganic Chemistry, 2009, 48, 11399-11406.	1.9	21
52	Observation of a Fano Resonance in Photoemission. Physical Review Letters, 1999, 82, 2971-2974.	2.9	19
53	Spin density in a triazole-nitronyl-nitroxide radical presenting linear ferromagnetic interactions: role of hydrogen bonding. Chemical Physics, 1999, 250, 23-34.	0.9	19
54	Electronic structure of predicted endohedral fullerenes An@C40 (An=Thâ€“Md). Computational and Theoretical Chemistry, 2013, 1013, 70-77.	1.1	19

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55	Interaction between zigzag single-wall carbon nanotubes and polymers: A density-functional study. Journal of Chemical Physics, 2005, 122, 214710.	1.2	18
56	DFT study of structural and vibrational properties of guanidinium derivatives. Computational and Theoretical Chemistry, 2009, 907, 16-21.	1.5	15
57	CHx adsorption (x = 1â€“4) and thermodynamic stability on the CeO2(111) surface: a first-principles investigation. RSC Advances, 2014, 4, 12245.	1.7	15
58	Quantum confinement effects in gallium nitride nanostructures:ab initioinvestigations. Nanotechnology, 2009, 20, 425401.	1.3	14
59	A DFT Study of the Energetical and Structural Landscape of the Tetrahedral to Squareâ€Planar Conversion of Tetrahalide Complexes of Copper(II)Â. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 1740-1750.	0.6	12
60	Guanidinium Formate Decomposition on the (101) TiO₂-Anatase Surface: Combined Minimum Energy Reaction Pathway Calculations and Temperature-Programmed Decomposition Experiments. Journal of Physical Chemistry C, 2011, 115, 1195-1203.	1.5	12
61	Brillouin zone folding and Fano resonances in commensurate rare gas monolayers observed in photoemission. Surface Science, 2000, 454-456, 483-488.	0.8	9
62	The Creutzâ^'Taube Complex Revisited: DFT Study of the Infrared Frequencies. Inorganic Chemistry, 2008, 47, 11269-11277.	1.9	9
63	DFT study of crystalline nitrosyl compounds. Zeitschrift Fur Kristallographie - Crystalline Materials, 2008, 223, 329-333.	0.4	7
64	Early transition metal dopants in cuprous oxide: To spin or not to spin. Current Applied Physics, 2013, 13, 1707-1712.	1.1	6
65	Enhancing Hydrophilicity of Anatase TiO₂ Surfaces by Deposition of Alkaline Earths: The Case of Ca. Journal of Physical Chemistry C, 2013, 117, 26013-26020.	1.5	6
66	Molecular adsorption and methanol synthesis on the oxidized Cu/ZnO(0001) surface. Surface Science, 2015, 641, 97-104.	0.8	6
67	Crystal structures and electronic properties of haloform-intercalatedC60. Physical Review B, 2002, 66, .	1.1	4
68	Density-functional calculations of Esterel twinning in quartz. Physical Review B, 2007, 76, .	1.1	4
69	Density functional calculations of polysynthetic Brazil twinning in Î±-quartz. Acta Crystallographica Section A: Foundations and Advances, 2012, 68, 359-365.	0.3	4
70	Fast full-field modulation transfer function analysis for photographic lens quality assessment. Applied Optics, 2021, 60, 2197.	0.9	4
71	Tailoring magnetic anisotropy by graphene-induced selective skyhook effect on 4f-metals. Nanoscale, 2022, 14, 7682-7691.	2.8	4
72	Evolution of the Electronic and Geometric Structure of Size Selected Pt and Pd Clusters on Ag(110) Observed by Photoemission. Materials Science Forum, 1996, 232, 51-66.	0.3	3

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73	Aluminium adsorption on Ir(111) at a quarter monolayer coverage: A first-principles study. Applied Surface Science, 2008, 254, 7655-7658.	3.1	3
74	Plutonium complexes in water: new approach to ab initio modeling. Radiochimica Acta, 2021, 109, 327-342.	0.5	2
75	Long-Lived Light-Induced Metastable States in trans-[Ru(NH3)4(H2O)NO] Cl3Ã—H2O and Related Compounds.. ChemInform, 2005, 36, no.	0.1	1
76	Publisher's Note: Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation [Phys. Rev. B77, 125423 (2008)]. Physical Review B, 2008, 77, .	1.1	1
77	Fano spectroscopy of impurities and clusters on solid surfaces. Journal of Electron Spectroscopy and Related Phenomena, 2002, 124, 195-210.	0.8	0
78	Comparison of experimental and theoretical results for the structure and elastic properties of moganite. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 279-286.	0.4	0
79	Density functional theory calculations of merohedric twinning in KLiSO₄. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 211-217.	0.4	0
80	Firstâ€principles study on the plutonium ions interaction with diamide molecules in acid solutions. International Journal of Quantum Chemistry, 2021, 121, e26681.	1.0	0
81	Wetting of Paracetamol Surfaces Studied by DMol3-COSMO Calculations. , 2011, , 37-46.		0